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POTENTIAL APPLICATIONS OF COMPUTATIONAL FLUID DYNAMICS TO BIOFLUID ANALYSIS

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SUMMARY

Computational fluid dynamics has been developed to the stage where it has become an indispensable part of aerospace research and design. In view of advances made in aerospace applications, the computational approach can be used for biofluid mechanics research. In the present paper, several flow simulation methods developed for aerospace problems are briefly discussed for potential applications to biofluids, especially to blood flow analysis.

INTRODUCTION

To date major advances in computational fluid dynamics (CFD) have been made in aerospace engineering. With the advent of supercomputers as well as the development of fast algorithms, computational flow simulations have become a practical means for aerospace designs. Therefore, it will be of considerable benefit to medical researchers to extend this CFD technology to biofluid analysis. One of the important areas of biofluid mechanics deals with blood flow, such as heart and blood vessel problems, which is relevant to cardiovascular diseases and their treatment. Understanding the flow phenomena by numerical simulations will be of significant value toward finding treatments for these problems. Therefore, the potential payoff to human health will be tremendous.

Blood flow is very complicated in many respects: The fluid may exhibit significant non-Newtonian characteristics locally and the geometry is usually very complicated. For instance, the human aorta has large curvatures combined with very irregular lumen cross sections and the walls are elastic and change shape (about a 10% increase in diameter during the systole). In an artificial organ, as red blood cells go through high-shear turbulence

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regions, they may be damaged; the downstream region of an artificial heart valve is an example. The flow is unsteady, possibly periodic, and very viscous and incompressible. This problem is very much interdisciplinary and an attempt for a complete simulation would be a very formidable task. However, an analysis based on a simplified model may provide much needed physical insight into the blood flow analysis. For a more comprehensive study on blood flow, a large number of publications are available (refs. 1-10) and is not reviewed here.

In the recent past, viscous incompressible flow solvers have been developed at NASA Ames Research Center. This research was motivated from realistic needs for three-dimensional simulations of aerospace applications (refs. 11-14). Naturally, computational efficiency has been of primary importance in addition to accuracy and robustness. The formulation is based on a Newtonian fluid assumption. However, since the governing equations are solved in a generalized coordinate system, viscosity is allowed to vary in space and time. These flow solvers can be applied to current blood flow problems, such as flow through an artificial heart (ref. 9), pulsatile flow in arterial bifurcations (ref. 6) and flow in aneurysms (ref. 7). A full simulation of viscoelastic flow is very difficult because of the nonlinearities of the fluid (ref. 5). However, as a first step toward full simulations, non-Newtonian effects of the blood flow can be simplified by a constitutive model for viscous stresses.

In the present paper, viscous incompressible flow CFD methods will be discussed for a potential extension to blood flow problems. The focus is on flow solvers recently developed by the authors, and on relevant features pertaining to blood flow simulations.

FORMULATION

Unsteady, three-dimensional, viscous, incompressible flow with constant density is governed by the following Navier-Stokes equations:

continuity equation

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

momentum equation

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

where, t is the time, x_i the Cartesian coordinates, u_i the corresponding velocity components, p the pressure, and τ_{ij} the viscous stress tensor. Here, all variables are nondimensionalized by a reference velocity and length scale.

To close the governing equations (1) and (2), the viscous stress tensor is modeled by a constitutive relation. For a Newtonian fluid, this can be written as

$$\tau_{ij} = 2\nu S_{ij} - R_{ij} \tag{3}$$

Here, ν is the kinematic viscosity, S_{ij} is the strain rate tensor, and R_{ij} is the Reynolds stresses. The strain rate tensor is defined by

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{4}$$

Various levels of closure models for R_{ij} are possible (ref. 15). If turbulence is simulated by an eddy viscosity model, the viscous stress tensor can be replaced by the following form:

$$\tau_{ij} = 2\nu_T S_{ij} \tag{5}$$

where ν_T is the effective total viscosity. Therefore, the present formulation allows variable viscosity which can be represented by a time-dependent constitutive relation. Non-Newtonian effects of blood can be included in a simple manner by an equation of state for ν_T. In a more sophisticated approach, a currently used differential model (ref. 5) for τ_{ij} ; namely,

$$\frac{D}{Dt}\tau_{ij} = f(t, p, S_{ij}, \text{material}) \tag{6}$$

can be incorporated in the analysis. This equation can be solved in a decoupled mode from the governing equations by lagging the time advancement by one step. In the remainder of this paper, our discussion will be limited to an algebraic expression as in Equation (5).

The geometric variation for blood flow computations is diverse and naturally the computational approach has to take this into account. To perform calculations on three-dimensional, arbitrarily shaped geometries, the following generalized independent variables are introduced which transform the physical coordinates into general curvilinear coordinates

$$\begin{aligned} \tau &= t \\ \xi_i &= \xi(x, y, z, t) \end{aligned} \tag{7}$$

Applying the transformation to the governing equations yields a generalized form of the incompressible Navier-Stokes equations cast in curvilinear coordinates. Various simplifications can be made on these equations depending on the geometry and the boundary-layer thickness. For instance, in many problems of external aerodynamics where the viscous

region is confined to a thin region, the Navier-Stokes equations are often simplified by a thin-layer approximation or by a parabolic form. For internal flows, such as the blood flow in the human body, viscous effects are important in the entire flow field. Therefore, the set of governing equations need to be solved in their complete form.

SOLUTION METHODS

A major problem in solving the incompressible Navier-Stokes equations comes from the lack of a pressure term in the continuity equation. In realistic three-dimensional applications, satisfying continuity in a reasonable amount of computing time becomes a primary issue. Various methods of resolving this problem have been developed (ref. 15). However, the present discussion is limited to a primitive variable formulation in generalized curvilinear coordinates. In this section, three flow solvers recently developed by the authors are summarized to suggest a way of extending this type of computational tool to blood flow simulations. Derivation of equations and algorithmic details can be found in full-length versions of the authors' publications (refs. 11-14). Other numerical methods developed in the past for simulating viscous incompressible flows can be found in the literature (see (ref. 15) for a review).

Pseudocompressibility method

Recent advances in the state of the art in CFD have been made in conjunction with compressible flow computations. Therefore, it is of significant interest to be able to use some of these compressible flow algorithms. To do this, the artificial compressibility method (ref. 16) can be used. In this formulation, the continuity equation is modified by adding a time derivative of the pressure term resulting in

$$\frac{1}{\beta}\frac{\partial p}{\partial t} + \frac{\partial u_i}{\partial x_i} = 0 \tag{8}$$

where β is a pseudocompressibility coefficient. Together with the unsteady momentum equations, this forms a hyperbolic-parabolic type of time-dependent system of equations. This method was originally intended for the steady-state computation of incompressible flow (refs. 11 and 12). However, by introducing a pseudo-time iteration, this can be made time-accurate (refs. 14 and 17).

By constructing a pseudocompressible form of the governing equations, fast, implicit schemes developed for compressible flows, such as the approximate-factorization scheme (ref. 18), can be implemented. Based on this approach,

a computer code (INS3D (ref. 11)) has been written for obtaining steady-state solutions. The spatial discretization uses second-order central differencing with additional numerical dissipation terms. This code has been validated and applied to numerous three-dimensional problems (refs. 11, 12, 19, and 20).

To obtain time-accurate solutions using the pseudocompressibility formulation, it is necessary to satisfy continuity at each time step by subiteration in pseudo-time. To use a large time step in the pseudo-time iteration, an upwind differencing scheme based on flux-difference splitting is used combined with an implicit line relaxation scheme. This removes the factorization error and the need for numerical dissipation terms. A second code (INS3D-UP) based on this method has been validated and excellent results have been obtained (ref. 14).

Fractional-step method

The fractional-step method is another approach that can be used for time-dependent computations of the incompressible Navier-Stokes equations. Here, the discretized equations are advanced in time by decoupling the solution of the momentum equation from that of the continuity equation. The common application of this method is done in two steps. The first step is to solve for an auxiliary velocity field using the momentum equation in which the pressure-gradient term is approximated by its value at the previous time step. In the second step, the pressure, which maps the auxiliary velocity onto a divergence-free velocity field, is computed. Various other operator splittings can be adopted by treating the momentum equation as a combination of convection, pressure, and viscous terms.

A third flow solver (INS3D-FS) based on this approach using a staggered grid has been developed (ref. 13). The governing equations are discretized conservatively using finite volumes. Rather than choosing the Cartesian velocity components as dependent variables, the volume fluxes over the faces of the computational cells are used. They are equivalent to the contravariant velocity components described in a staggered grid. This procedure, combined with accurate and consistent approximations of the geometric quantities, satisfies the discretized mass conservation equation. In the second step, a novel four-color scheme is devised for solving the resulting Poisson equation for the pressure correction. Several computational results have been compared with experiments and other numerical solutions in reference 13.

COMPUTATIONAL PROCEDURE

Grid generation

Commonly used grid topologies can be classified basically into three different types, namely, O-, C- and H-grids. In blood flow applications, the blood vessels have tubular cross sections and can branch off into several smaller tubes. The flow can go through irregular passages and may encounter rapid turns and expansions as in an artificial heart (refs. 8 and 9). Naturally, computational simulation of these flows needs to be performed in more than one zone that are separated by geometric characteristics. For a multiple zone calculation, geometric continity is desirable for avoiding complicated interface procedures. Various grid generators are available in the literature.

To illustrate a possible way of generating a realistic grid, the geometry of a glass aneurysm model, proposed by Liepsch et al. (ref. 7), is chosen. Note that, by combining the two H-grids, the grid in the cavity is continuous with the grid in the main blood vessel. Figure 1(a) shows that the grid for the physical domain and figure 1(b) shows the grid for the computational domain (generated by L. Chang: unpublished note). Here, the circular cross sections are mapped by an H-grid. This topology is very flexible in clustering the grid points in the area of interest; however, it does so at the expense of introducing singular points. These singularities are hidden in the corner of the solid boundary and can easily be handled by explicit boundary conditions.

Computed examples

The three flow solvers just described have been validated by computing basic fluid dynamics problems (refs. 11-13). A few examples are listed in this section for demonstrating the capability of those solvers for potential applications to blood flow problems.

Bifurcation is an important blood flow problem, since a low-speed recirculating region and local regions of high shear stress may play an important role in the formation of atherotic plaques and thrombi as well as releasing hemoglobin in the blood stream. As an idealization of a branching human circulatory system, a numerical solution of a 90° bifurcation problem (ref. 6) is shown in figure 2. This result is obtained using the INS3D-UP code (ref. 15). A more realistic geometry can be modeled by a grid similar to the aneurysm shown in figure 1.

In figure 3, the time evolution of a two-dimensional cavity flow is shown by time dependent stream function contours. This result is obtained by the INS3D-FS code (ref. 13). This example illustrates the potential of extending the flow solver to an aneurysm analysis.

As an example of how the present CFD capabilities are being used in real world applications, work related to the Space Shuttle main engine (SSME) flow simulation (refs. 19 and 20) is briefly discussed here. The geometric complexity of the SSME power head is comparable to blood flow problems, such as flow in an artificial heart. In the SSME staged combustion cycle, the fuel is partially burned at very high pressure and relatively high temperature in the preburners. The resulting hot gas is used to drive the turbine and is then discharged from the gas turbine to the annular turnaround duct with a 180° U-turn before it diffuses into the fuel bowl. Flow through this assembly was simulated using INS3D code. The flow in the U-turn is especially interesting when the flow is turbulent because the turbulence structure is greatly influenced by streamline curvature. Therefore, in this case, it is necessary to incorporate strong curvature effects in the turbulence modeling. For the present paper, a length scale determined by the point of minimum vorticity is incorporated into an extended Prandtl-Karmann mixing-length theory. The combination of these automatically account for the curvature effect. Full details of this model are given in reference (ref. 21). In figure 4(a), the grid in the 180° turn region is shown. In figures 4(b)-4(i), computed velocity profiles using this algebraic turbulence model at $Re=10^5$ are compared with experiment (ref. 22). Considering the difficulties associated with curvature effect modeling, the results are very promising.

Postprocessing

Three-dimensional simulation of realistic flow produces an avalanche of data. Therefore, fast postprocessing tools are necessity for analyzing the data. Various three-dimensional graphic softwares have been developed in parallel with supercomputers. Graphics work can be performed on a work station independently or interactively with the main supercomputer. This provides an invaluable means in interpreting and understanding the results of the computation. Further details of the recent development in postprocessing can be found in the references cited (refs. 23 and 24).

CONCLUDING REMARKS

This paper presents a potential procedure of applying incompressible Navier-Stokes flow-solvers to blood flow problems. Computed examples on several generic problems

relevant to blood flow are presented. For problems related to large blood vessels, the present Newtonian formulation is an acceptable approximation for gaining insight into the flow physics involved. However, for a more complete and accurate analysis, it will be required to model the non-Newtonian effect as well as the transition and turbulence effects. Despite the limitation on physical models, the successful application of the incompressible Navier-Stokes solvers to the SSME analysis and redesign, provides an example of present CFD capabilities. These capabilities can be integrated into the blood flow analysis, since similar approximations to the physics can be made in that case.

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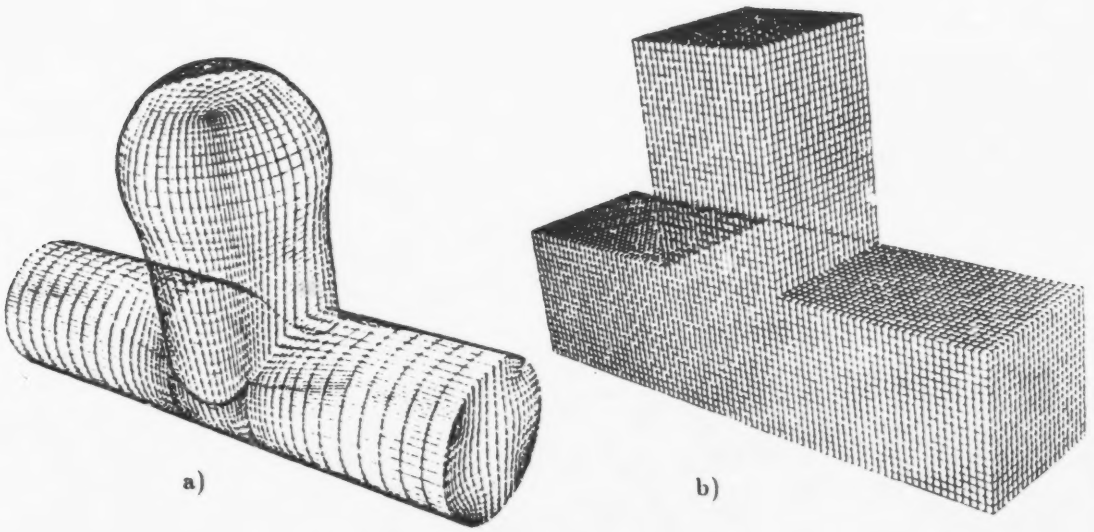

Fig. 1 Model geometry of an aneurysm: a) physical domain,
b) computational domain

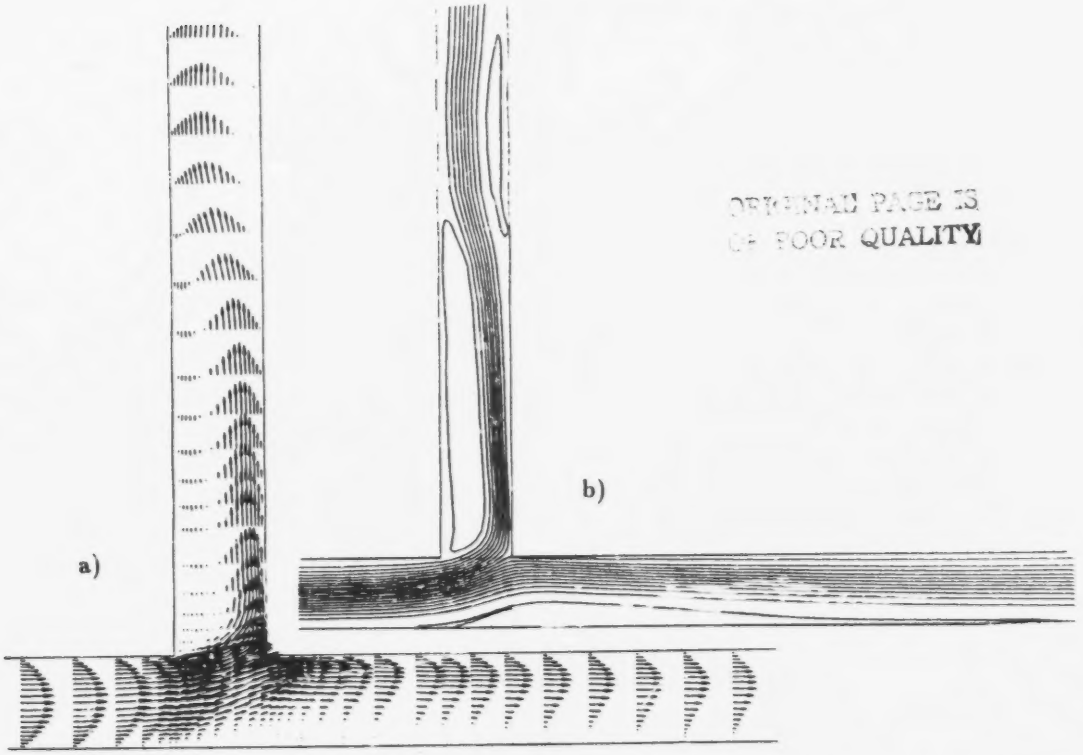

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Fig. 2 Numerical solution of 90° bifurcation (Re=496, vertical flow = 44 % of total flow):
a) velocity vectors, b) stream function contours.

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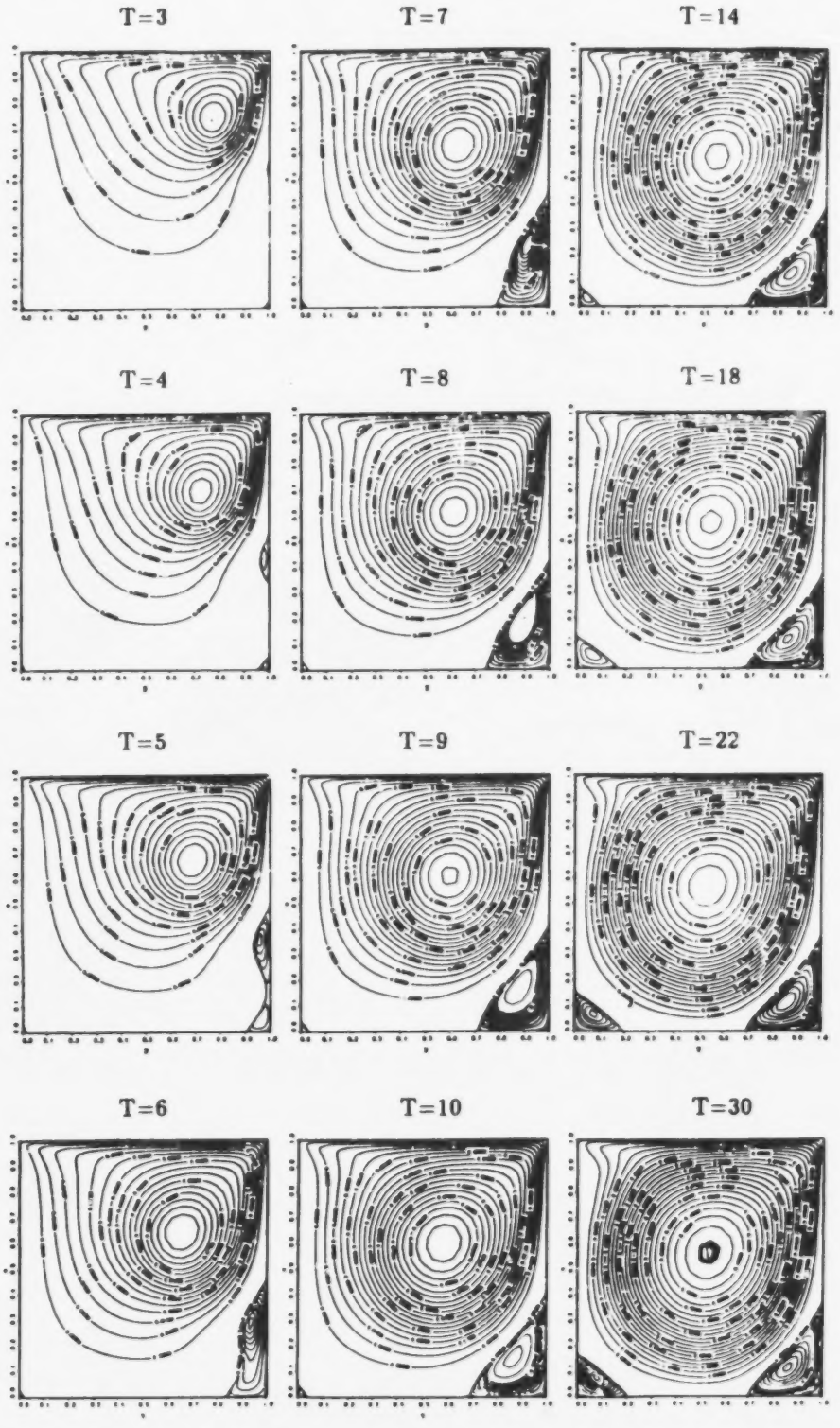

Fig. 3 Time evolution of stream function contours for a 2-D driven cavity at Re=1000.

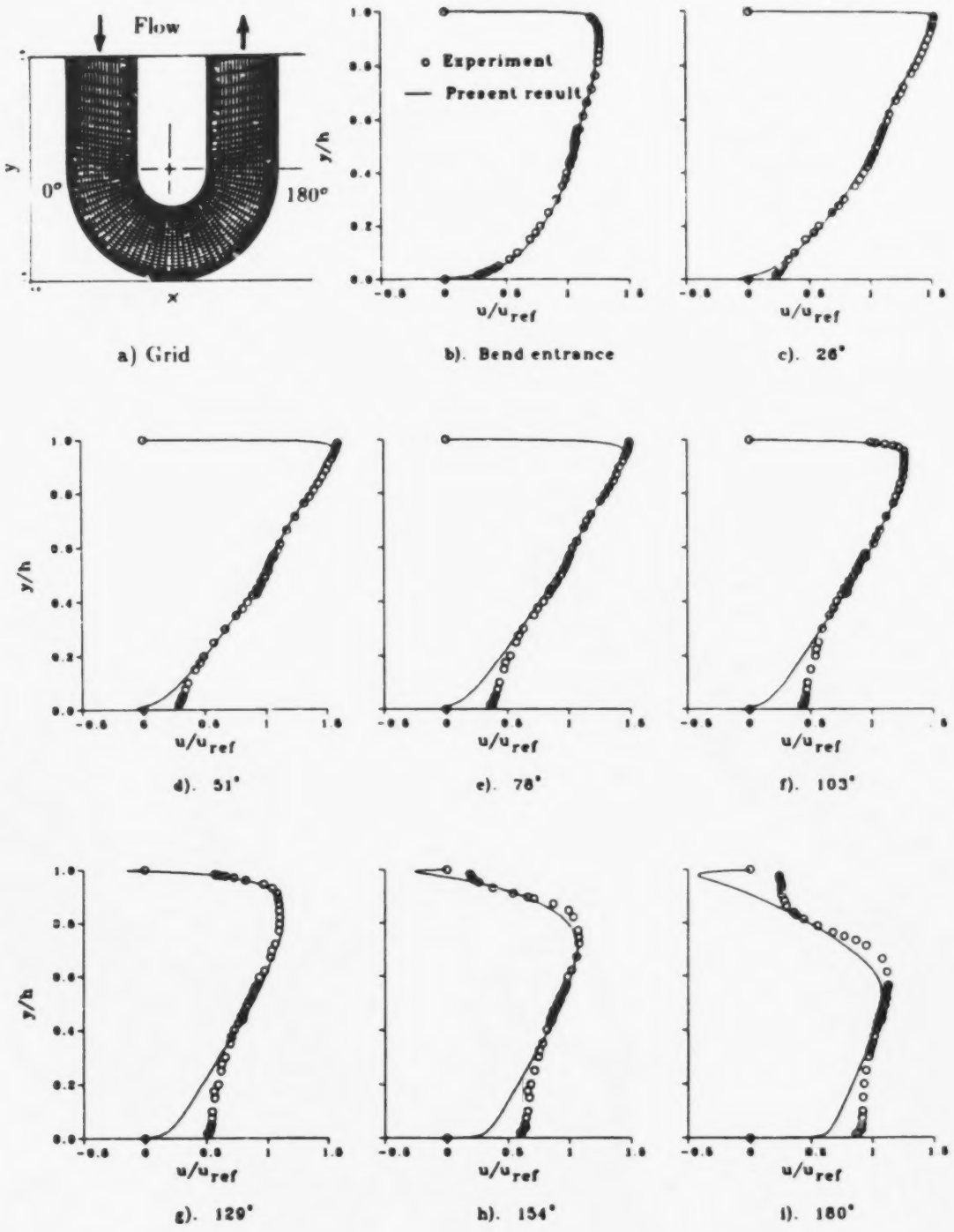

Fig. 4 Grid and normalized streamwise velocities for an axisymmetric U-turn at Re=10^5.

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16. Abstract

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